Compact QED under scrutiny: it's first order

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We report new results from our finite size scaling analysis of 4d compact pure U(1) gauge theory with Wilson action. Investigating several cumulants of the plaquette energy within the Borgs-Kotecky finite size scaling scheme we find strong evidence for a first-order phase transition and present a high precision value for the critical coupling, β_T in the thermodynamic limit.

1. INTRODUCTION

The nature of the phase transition in compact QED has been under debate for long time. We have addressed this problem in high statistics runs to reach a final conclusion in that matter. An important ingredient of our approach is the finite size scaling (FSS) theory à la Borgs-Kotecky (BK) first established a long time ago in the context of strong first order phase transitions [1–3]. According to BK the finite volume partition function at temperature β in finite volumes with periodic boundary conditions (neglecting interfacial contributions) has the remarkably simple form $Z = e^{-Vf(\beta)} = e^{-Vf_1(\beta)} + e^{-Vf_2(\beta)+\ln(X)}$. The functions $f_1(\beta)$ and $f_2(\beta)$ denote bulk free energy densities in the two coexisting phases 1 and 2. X stands for the asymmetry parameter which is nothing but the relative phase weight in the probability distribution $P(E)$.

A heuristic extension of the BK ansatz to weak first order transition was demonstrated for the 3d 3-state Potts model [4]. The conclusion of our work is based on a validation of BK by perturbative analysis as well as independent ab initio determinations of the gap characteristics.

2. SIMULATION DETAILS

We consider 4d pure U(1) gauge theory with Wilson action $S = -\beta \sum_{n,\nu>\mu} \cos(\theta_{\mu\nu}(n))$, where β represents the Wilson coupling and $\theta_{\mu\nu}(n)$ the plaquette angle. We use a lattice of volume $V = L^4$ with periodic boundary conditions.

We have implemented three different algorithms for generating the U(1) gauge field configurations: (a) a local Metropolis (Metro), updating each link separately, (b) a global hybrid Monte Carlo algorithm (HMC) and (c) a combination of the multicanonical and the hybrid Monte Carlo algorithm (MHMC). For details we refer to Refs. [5,6]. The cumulative number of generated configurations at each lattice size L is $> 5 \times 10^6$. We measure the number of tunneling events (flips) as control parameter for the mobility of the algorithms and the integrated plaquette autocorrelation time τ_{int} which controls the statistical quality of each single Markov chain. Runs differing by coupling, algorithm, HMC parameters or by weight function are considered as independent. Our simulation parameters are listed in Table 1.

3. CUMULANTS

Based on the plaquette operator

$$E = \frac{1}{6V} \sum_{n,\nu>\mu} \cos(\theta_{\mu\nu}(n)), \tag{1}$$

we consider the following cumulants:

$$\begin{aligned} C_v(\beta, L) &= 6V \left(\langle E^2 \rangle - \langle E \rangle^2 \right), \\ U_2(\beta, L) &= 1 - \frac{\langle E^2 \rangle}{\langle E \rangle^2}, \\ U_4(\beta, L) &= \frac{1}{3} \left(1 - \frac{\langle E^4 \rangle}{\langle E^2 \rangle^2} \right). \end{aligned}$$

In addition to their derivatives with respect to β we measure higher derivatives of the free energy

Table 1
Simulation details. The HMC subscript denotes length of trajectory.

L	β	algorithm	#conf$\times 10^6$	#flips	τ_{int}
6	1.001700	Metro	11.20	21170	104(2)
	1.001500	Metro	9.80	18300	104(2)
	1.001600	HMC	2.48	3577	130(5)
	1.001772	MHMC	4.90	7444	102(2)
8	1.007370	Metro	2.79	2512	304(16)
	1.007370	HMC_2	1.25	274	1256(196)
	1.007370	HMC_4	1.25	554	649(73)
	1.007370	HMC_6	1.25	698	450(42)
	1.007370	HMC_8	1.25	846	390(33)
	1.007370	HMC_9	1.25	907	339(27)
	1.007370	HMC_{10}	1.25	921	328(26)
	1.007370	HMC_{11}	1.25	929	345(28)
	1.007370	HMC_{12}	1.25	911	363(30)
	1.007370	HMC_{13}	1.25	932	355(29)
	1.007370	HMC_{14}	1.25	854	382(33)
	1.007370	HMC_{16}	1.25	856	399(35)
	1.007370	HMC	1.44	1058	379(30)
	1.007337	MHMC	6.36	5179	240(7)
10	1.009300	Metro	4.37	1770	784(52)
	1.009400	Metro	7.44	3104	775(35)
	1.009300	HMC_9	1.00	294	948(144)
	1.009300	HMC_{11}	1.00	350	897(132)
	1.009300	HMC_{15}	1.00	353	1060(170)
	1.009300	HMC_{17}	1.00	344	831(118)
	1.009300	HMC_{19}	1.00	340	894(132)
	1.009300	MHMC	2.61	1318	412(56)
12	1.010143	Metro	3.62	569	2406(304)
	1.010143	Metro	5.88	916	2058(189)
	1.010143	Metro	1.75	315	2576(486)
	1.010143	Metro	1.87	308	2098(345)
	1.010143	MHMC	1.30	403	734(86)
	1.010143	MHMC	2.18	702	689(60)
14	1.010598	Metro	3.90	215	5980(1150)
	1.010600	Metro	6.52	395	7480(1240)
	1.010568	HMC	0.57	26	12500(9000)
	1.010568	MHMC	0.83	169	1070(190)
	1.010568	MHMC	3.80	725	1380(130)
16	1.010753	Metro	5.42	75	22900(9000)
	1.010800	Metro	5.55	93	25400(6800)
	1.010753	MHMC	0.60	66	1980(560)
	1.010753	MHMC	0.63	77	1850(500)
	1.010753	MHMC	1.63	151	1770(290)
	1.010753	MHMC	3.39	424	1800(200)
18	1.010900	MHMC	0.38	13	9900(7900)
	1.010900	MHMC	0.63	20	10000(6800)
	1.010900	MHMC	0.98	58	5800(2200)
	1.010900	MHMC	3.79	272	4700(820)

density $(-1)^{n+1}\kappa_n(\beta,L) = \frac{\partial^n f(\beta,L)}{\partial\beta^n}$. Introducing the central moments $\mu_n = V^{n-1}\left\langle (E - \langle E\rangle)^n\right\rangle$ we can write them as

$$
\begin{aligned}
\kappa_3 &= \mu_3, \\
\kappa_4 &= \mu_4 - 3V\mu_2^2, \\
\kappa_5 &= \mu_5 - 10V\mu_2\mu_3, \\
\kappa_6 &= \mu_6 - 15V\mu_2\mu_4 - 10V\mu_3^2 + 30V^2\mu_2^3.
\end{aligned}
$$

For each of the ten cumulants the location (β_κ, κ) of its rightmost extremum is determined by reweighting the measured probability distribution $P(E)$ to different couplings β. To calculate the estimates of our cumulants at each lattice size L we proceed in two steps: i) we determine the error of each individual run performing a jackknife error analysis by subdivision of the run into ten blocks; ii) we calculate the final result by χ^2-fitting these individual results to a constant.

4. FINITE SIZE SCALING

Let us consider the expansion of the pseudocritical coupling for C_v; in the BK representation it is given by

$$\beta_{Cv}(V) = \beta_{Cv}(\infty) + \sum_{k=1}^{k_{max}} B_k V^{-k}. \qquad (2)$$

In order to expose systematic effects in the fit parameter $\beta_{Cv}(\infty)$, we vary both, the fit range within $L_{min} \leq L \leq 18$ and the truncation parameter k_{max}. Table 2 displays a remarkable stability pattern both for β_{Cv} and B_1 supporting the validity of the V^{-1}-expansion. Averaging the best fit couplings to a constant we obtain $\beta_{Cv}(\infty) = 1.0111310(62)$. Performing the same analysis for all ten cumulants yields an average infinite volume transition coupling

$$\beta_T = 1.0111331(21). \qquad (3)$$

Table 2
Transition couplings $\beta_{Cv}(\infty)$ fitted to Eq (2). Best fits are in bold face letters.

L_{min}	k_{max}	χ^2_{dof}	$\beta_{Cv}(\infty)$	B_1
14	1	1.03	1.0111241(13)	-18.95(14)
12	1	1.09	1.0111144(55)	-18.24(21)
	2	**0.19**	**1.0111315(57)**	**-19.96(53)**
10	1	12.7	1.0110945(147)	-17.18(37)
	2	**0.13**	**1.0111283(25)**	**-19.63(15)**
	3	**0.21**	**1.0111319(62)**	**-20.06(65)**
8	1	108	1.0110474(349)	-15.33(50)
	2	2.14	1.0111159(69)	-18.70(25)
	3	**0.11**	**1.0111309(25)**	**-19.94(17)**
	4	**0.21**	**1.0111309(22)**	**-19.94(10)**
6	1	970	1.0109389(913)	-12.38(56)
	2	37.1	1.0110792(218)	-16.84(41)
	3	1.25	1.0111199(55)	-19.02(22)
	4	**0.10**	**1.0111316(11)**	**-20.02(6)**

Analogously the expected scaling of the maxima of the specific heat yields a prediction for the infinite volume gap G

$$\begin{aligned}\frac{C_{v,max}(V)}{6V} &= \frac{1}{4}G^2 + \sum_{k=1}^{\infty} C_k V^{-k} \\ G &= 0.026721(59). \end{aligned} \tag{4}$$

Scaling of the Binder cumulant yields

$$\begin{aligned}U_{4,min} &= U + \sum_{k=1}^{\infty} A_k V^{-k} \\ U &= -5.816(27)\ 10^{-4}. \end{aligned} \tag{5}$$

From $B_1 = -\frac{\ln(X)}{6G}$ we can derive an asymmetry $\ln(X) = 3.21(10)$.

5. CONSISTENCY CHECKS

An independent leading order perturbative lattice calculation confirms the value of $\ln(X)$ without relying on the validity of the BK ansatz [7]. In the Coulomb phase the partition function can approximately be written as

$$Z \simeq \left(\frac{2\pi}{e_R^2}\right)^{-\frac{3}{2}(V-1)} V^{\frac{1}{2}} {\prod_p}' \left[\sum_\mu 2(1-\cos p_\mu)\right]^{-1},$$

leading to the free energy $F_2 = \ln Z = -\frac{3}{2}(V-1) \ln(\frac{2\pi}{e_R^2}) + 2\ln L - {\sum_p}' \ln \sum_\mu 2(1-\cos p_\mu)$. The summation over all momenta p_μ can be done for asymptotically large L as ${\sum_p}' \ln \sum_\mu 2(1 - \cos p_\mu) = aV + 2\ln L - b + \mathcal{O}(L^{-2})$ with parameters $a = 1.999708$ and $b = 1.701216$ that can be numerically computed to arbitrary precision. With $F_2(\beta, L) = V f_2(\beta) + \Delta F_2(\beta, L)$ we obtain for the Coulomb phase finite size correction $\Delta F_2 = b + \frac{3}{2}\ln(2\pi/e_R^2) = 3.15(8)$. e_R is taken from a very accurate measurement of the renormalized fine structure constant at the phase transition $\alpha_T = e_R^2/4\pi = 0.19(1)$ [8]. Note that the logarithmic correction cancels out for the 4d symmetric system with periodic boundary conditions.

One can argue that the leading finite size effects in the confined phase due to 0^{++} gaugeballs and string states are at least 3 respectively 6 orders of magnitude smaller than ΔF_2 on a lattice as small as $L = 16$ [7]. Thus we neglect these contributions and obtain, in perfect agreement, an asymmetry parameter $\ln(\hat{X}) = \Delta F_2 = 3.15(8)$.

Furthermore our very accurate value of β_T (Eq (3)) admits a direct measurement of latent heat and Binder cumulant, performing metastable simulations at β_T on lattice sizes up to 32^4 [9]. Denoting the energy peaks of the probability distribution in the confined and Coulomb phases by $E_1(L)$ and $E_2(L)$ we fit their continuum limit values $E_i = E_i(\infty)$ and find

$$\hat{G} = E_2 - E_1 = 0.026685(54), \tag{6}$$

$$\hat{U} = -\frac{(E_2^2 - E_1^2)^2}{12 E_2^2 E_1^2} = -5.777(16)\ 10^{-4}. \tag{7}$$

Both values are in perfect agreement with the BK results from Eqs (4,5).

6. SUMMARY AND CONCLUSION

All cumulants investigated in our high statistics analysis at L=6,8,10,12,14,16,18 can be described by BK first-order FSS. Ab initio measurements *confirm* the FSS results for the infinite volume gap G, the Binder cumulant U and the asymmetry $\ln(X)$. The non vanishing values for G and U lead to the conclusion that the phase transition in compact 4d $U(1)$ theory with Wilson action is first-order.

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